

Optical conductivity of one-dimensional doped Hubbard-Mott insulator

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We study the optical response of a strongly correlated electron system near the metal-insulator transition using a mapping to the sine-Gordon model. With semiclassical quantization, the spectral weight is distributed between a Drude peak and absorption lines due to breathers. We calculate the Drude weight, the optical gap, and the lineshape of breather absorption.

Optical absorption is one of the basic tools in studies of the spectral properties of strongly correlated electron systems^{1,2,3}. An important class of such systems is comprised of one-dimensional conductors such as ladder compounds, organic metals and stripes in high T_c cuprates. The electron-electron interaction in these low-dimensional systems is known⁵ to result in spin-charge separation and formation of a Luttinger liquid or the Mott-Hubbard insulator (MHI). The MHI occurs at commensurate filling fractions and is characterised by an energy gap in the charge sector. In this case, optical absorption exhibits a threshold at twice the gap energy. As the Fermi level shifts above the gap, the system conducts, with profound changes to the optical absorption spectrum. The optical conductivity summarizes this behavior: $\sigma(\omega) = D 2\pi\delta(\omega) + \sigma_{\text{reg}}(\omega)$, with the Drude weight $D = 0$ in the insulating phase, and a regular part σ containing contributions from pair excitations and bound states, or excitons⁶.

The simplest model where the MHI phase occurs is the Hubbard model with an on-site repulsion. In the commensurate phase the spectrum of the optical absorption consists of a broad feature lying in the particle-hole continuum^{7,8,9}. In the more realistic extended Hubbard model, the excitation spectrum generally consists of both the particle-hole continuum and bound states (excitons)^{10,11}. Numerical studies of the extended Hubbard model with nearest- and next-nearest neighbor repulsions¹² show the emergence of a sharp exciton peak, which becomes a dominant feature when the repulsion is sufficiently strong.

In addition to the numerical analysis of the problem a mapping to the continuous sine-Gordon (SG) model can be considered⁶. The exciton peaks are seen in the sine-Gordon approach as absorption on quantum "breather" modes of the model.

Much is known about the commensurate phase because of the integrable structure of the corresponding SG theory and the knowledge of its form-factors due to the Smirnov bootstrap (see¹² and refs therein). The incommensurate phase is much less studied with analytic results existing for the high frequency expansion of the optical conductivity in the absence of breathers⁶.

In this paper we report our results for the optical conductivity in the incommensurate phase in the presence of a large number of breathers, which corresponds to long-range interactions in the Hubbard chain¹¹. It is

known that in this limit the SG model can be analyzed semiclassically¹³. Using the semiclassical approach we calculate the optical absorption of a doped MHI as a function of frequency and the carrier density. Our analytic expression for the Drude weight (21) is found in an excellent agreement with a thermodynamic Bethe ansatz calculation. At high doping the optical weight is contained in the Drude peak and in a series of well resolved peaks at finite frequencies, corresponding to excitation of breathers. We calculate the positions of the peaks (19), and their shape (33). At low doping peaks merge in a narrow continuous band and we provide an analytic expression for the optical absorption in this case. Our results for one spatial dimension agree with experimental and theoretical evidences for the peaks in optical absorption at small energies near the metal-insulator transition in quasi 1D compounds and in higher dimensions^{1,3,4,15,16}.

The optical response of a doped MHI is described by the sine-Gordon model^{6,14}

$$\mathcal{L} = \frac{1}{2} \{ (\partial_t \phi)^2 - (\partial_x \phi)^2 \} + \frac{m^2}{\beta^2} \cos \beta \phi + h \frac{\beta}{2\pi} \partial_x \phi \quad (1)$$

where the charge and current densities read

$$\rho = \frac{\beta}{2\pi} \partial_x \phi, \quad j = -\frac{\beta}{2\pi} \partial_t \phi. \quad (2)$$

In Eq. (1) h is the chemical potential controlling the average density $\langle \rho(x) \rangle = \bar{\rho}$, and it is assumed that in the insulating phase $\bar{\rho} = 0$. The cosine term in Eq.(1) is related to Umklapp. The sine-Gordon coupling β is determined by the interactions of the lattice model⁵. For free fermions $\beta = \sqrt{8\pi}$. For infinite U Hubbard model $\beta = \sqrt{4\pi}$, which corresponds to the refermionization point, where the optical absorption can be found exactly¹⁷. Below, we will investigate the case of $\beta \ll 1$ when the number of breather modes is $\sim 8\pi/\beta^2$. The mass m is a characteristic energy scale for a breather excitation while the particle-hole continuum starts from energies $\sim 8m/\beta^2$.

By virtue of (2) the Kubo formula for the optical conductivity is written as

$$\sigma(\omega) = \left(\frac{\beta}{2\pi} \right)^2 \text{Im} \int_0^\infty dt e^{-i\omega t} G(t), \quad (3)$$

where

$$G(t) = \int dx \langle [\pi(x, t), \phi(0, 0)] \rangle. \quad (4)$$

and $\pi = \partial_t \phi$ is the canonically conjugate momentum for ϕ , such that $[\phi(x), \pi(y)] = i\delta(x - y)$.

It follows from (3) that $\sigma(\omega)$ satisfies a sum rule

$$\int_{-\infty}^{\infty} d\omega \sigma(\omega) = i \frac{\beta^2}{4\pi} \int dx \langle [\pi(x, 0), \phi(0, 0)] \rangle = 2\tau, \quad (5)$$

with $\tau = \beta^2/8\pi$. In the Tomonaga-Luttinger limit, $m = 0$ in (1), the sum rule (5) is saturated by the Drude weight $D = \tau/\pi$.

In the quasiclassical regime the case $\bar{\rho} = 0$ is very simple. Eq. (1) reduces to the Klein-Gordon model, with the ground state $\phi = 0$. The optical conductivity is calculated immediately

$$\sigma_{\text{KG}}(\omega) = \tau (\delta(\omega - m) + \delta(\omega + m)), \quad (6)$$

For a finite $\bar{\rho}$ the quasiclassical ground state found from the stationary SG equation under constraint $\langle \partial_x \phi \rangle = 2\pi\bar{\rho}/\beta$ is

$$\phi_0(x) = 2\beta^{-1} \text{am}(2K\bar{\rho}x) \quad (7)$$

where $\text{am}(x, k)$ is the Jacobi amplitude function¹⁸ with the elliptic index k . This index is found from the equation

$$m/\bar{\rho} = 2kK(k) \quad (8)$$

with the complete elliptic integral K . Henceforth we will drop the index k in the argument of the elliptic functions and use the conventions $k_1 = \sqrt{1 - k^2}$, $K(k) = K$, $K(k_1) = K'$, $E(k) = E$. The standard semiclassical approach requires the second variation of the action around the classical solution and an analysis of the spectrum of the resulting Gaussian action. It was, shown¹⁸ that this scheme encounters infrared divergences in higher orders of perturbation theory in β . An infrared stable formulation of the theory is achieved by a non-linear change of variables

$$\phi = \phi_0(x + \kappa^{-1}\beta\eta). \quad (9)$$

where $\kappa = 2\pi\bar{\rho}$. The new field variable $\eta(x, t)$ plays the role of the continuous "collective coordinate"¹⁹, which roughly corresponds to fluctuations in kinks' positions.

The linearized Lagrangian for the field η reads

$$\mathcal{L} = \frac{1}{2} w^2(x) \{ (\partial_t \eta)^2 - (\partial_x \eta)^2 \}. \quad (10)$$

where the weight function, w is defined as

$$w(x) = \frac{2K}{\pi} \text{dn} 2K\bar{\rho}x. \quad (11)$$

The spectrum of the Lagrangian (10) was analyzed in detail in¹⁸. The eigenmodes of (10) are the Bloch functions

$$\eta_q(x, t) = e^{iqx - i\omega_q t} \chi_q(x), \quad (12)$$

where q is the Bloch wave vector and χ is the modulating Bloch function with period $1/\bar{\rho}$.

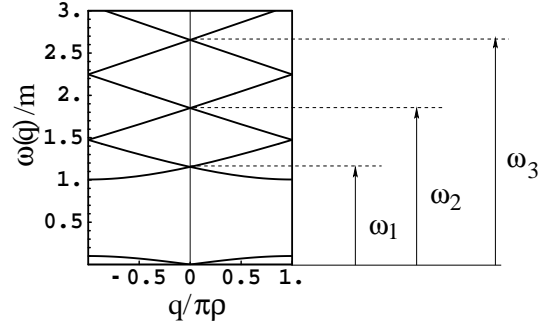


FIG. 1: Semiclassical result for the spectrum in the reduced Brillouin zone scheme for $\bar{\rho}/m = 0.14$. The first three allowed transitions are labeled ω_1, ω_2 and ω_3 .

These solutions are conveniently parametrized by a complex parameter α as follows. The Bloch wave vector and the eigenfrequency of the mode are given by

$$q = -i2\bar{\rho}KZ(\alpha) + \pi\bar{\rho}, \quad \omega = 2\bar{\rho}K \text{dn}(\alpha), \quad (13)$$

where $Z(\alpha)$ is the Jacobi Zeta function. The modulating Bloch function is

$$\chi_q(x) = C_\alpha e^{i\pi\bar{\rho}x} \vartheta_1\left(\pi\bar{\rho}x - \frac{\pi\alpha}{2K}\right) \vartheta_3^{-1}(\pi\bar{\rho}x). \quad (14)$$

Here the coefficient C_α is chosen to fulfill the normalization condition

$$\int dx w^2(x) \eta_\alpha^*(x) \eta_\beta(x) = \delta_{\alpha\beta}. \quad (15)$$

The quantized field $\eta(x, t)$ is then represented in the oscillator basis

$$\eta(x, t) = \sum_\alpha \left(\frac{\eta_\alpha(x)}{\sqrt{2\omega_\alpha}} e^{i\omega_\alpha t} b_\alpha^\dagger + h.c. \right) \quad (16)$$

with operators b, b^\dagger satisfying usual commutation relations $[b_\alpha, b_{\alpha'}^\dagger] = \delta_{\alpha\alpha'}$.

In the limit of small β the change of variables (9) can be linearized $\phi = \phi_0 + w\eta$, $\pi = w\dot{\eta}$ and from the normal mode expansion (16) and the Kubo formula (3) one obtains for the optical conductivity

$$\sigma(\omega) = \tau \sum_\alpha |F(\alpha)|^2 (\delta(\omega - \omega_\alpha) + \delta(\omega + \omega_\alpha)), \quad (17)$$

where the form factor

$$F(\alpha) = \frac{1}{\sqrt{L}} \int_0^L dx \eta_\alpha(x) w(x). \quad (18)$$

The selection rules for the form factors in (17) should allow only transitions between the states of zero wave vector in the reduced Brillouin zone scheme (see Fig. 1). This condition combined with (13) implies that the allowed indices α and the corresponding frequencies of the absorption lines satisfy

$$2iKZ(\alpha_n) = \pi(2n - 1), \quad \omega_n = (m/k) \text{dn} \alpha_n, \quad (19)$$

where $n = 1, 2, 3, \dots$ and $\alpha_n \in [0, iK']$. For the form factors we find

$$|F(\alpha_n)|^2 = \frac{\pi^2}{2K^2} \frac{\text{csch}^2 \left[\frac{i\pi\alpha_n}{2K} + iK'Z(\alpha_n) \right]}{\text{dn}^2 \alpha_n - \frac{E}{K}}. \quad (20)$$

The lowest frequency ω_1 can be associated with the optical gap. From Eq. (19) (see also Fig. 1) one finds that ω_1 is always greater than m and is an increasing function of $\bar{\rho}$. One has $\omega_1 \simeq m$ for $\bar{\rho} \ll m$ and $\omega_1 \simeq 2\pi\bar{\rho}$ for $\bar{\rho} \gg m$. The spacings between the peaks also increase with $\bar{\rho}$, from zero at $\bar{\rho} \rightarrow 0$ to $2\pi\bar{\rho}$ for $\bar{\rho} \gg m$. The amplitudes $|F(\alpha_n)|^2$ are rapidly decreasing functions of n . In the high density limit one finds $|F(\alpha_n)|^2 \sim n^{-2}(4\pi\bar{\rho}/m)^{-4n}$.

The Drude weight comes from the zero mode η_0 and is found to be

$$D = \frac{\tau}{\pi} |F_0|^2 = \frac{\tau\pi}{4EK} \quad (21)$$

Combined with definition (8) formula (21) gives the quasiclassical expression for the Drude weight as a function of the density of kinks. The following limiting cases allow for further simplifications:

1. *High density limit.* This limit corresponds to $k \rightarrow 0$ and $K, E \rightarrow \pi/2$. For the Drude weight we get $D \rightarrow \tau/\pi$, which is the result for the Tomonaga-Luttinger limit.
2. *Low density limit.* In this limit both k and E are close to unity. The Drude weight is then given by

$$D = \frac{\bar{\rho}}{2M_s}. \quad (22)$$

This result has a simple physical interpretation. In the limit of low density the kinks form a gas of weakly interacting non-relativistic particles. In an external electric field ε the motion of a particle is described by Newton's law $-iM_s\omega v = \varepsilon$ and the electric current is given by $j = -\bar{\rho}\varepsilon/(i\omega M_s)$. Analytic continuation of this expression gives Eq. (22).

To check the accuracy of these results we calculate the exact Drude weight from the thermodynamic Bethe ansatz²⁰. A comparison made in Fig. 2 shows an excellent agreement between the quasiclassics and the exact result.

Further analysis needs a different treatment of the cases of the high and the low density.

In the limit $\rho/m \rightarrow 0$ one has $K \rightarrow \infty$ so that both the weight of δ -functions in (17) and the spacings between them vanish. (In this limit one has $K' \rightarrow \pi/2$, $E \rightarrow 1$, $Z(\alpha) \rightarrow \tanh \alpha$, $\text{dn} \alpha \rightarrow \text{sech} \alpha$ and $\alpha_n \simeq -i(2n+1)\pi\bar{\rho}/m$, $\omega_n^2 = m^2 + [(2n+1)\pi\bar{\rho}]^2$.) As a result, the sequence of δ -functions merges to the continuous function

$$\sigma_{\text{reg}}(\omega) = \frac{\tau\pi\bar{\rho}}{|\omega|\sqrt{\omega^2 - m^2}} \frac{\vartheta(\omega^2 - m^2)}{\sinh^2 \frac{\pi}{2m}\sqrt{\omega^2 - m^2}} \quad (23)$$

Note the non-integrable singularity $\sigma(\omega) \sim (\omega - m)^{-3/2}$ at the threshold, which seemingly violates the sum rule

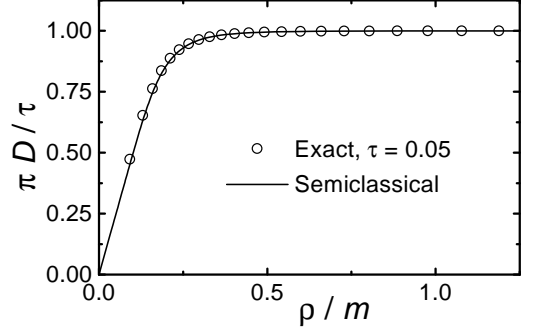


FIG. 2: Drude weight as a function of soliton density in the small τ limit. The solid line corresponds to the semiclassical result, Eqs. (8), (21). The exact values of the Drude weight calculated from the Bethe ansatz for $\tau = 0.05$ are shown by circles.

- (5). This signals that the low density limit requires special treatment. A careful analysis of the fluctuations in this limit²¹ leads to the formula

$$\sigma(\omega) = \frac{\tau|\omega|}{\pi m \sqrt{\omega^2 - m^2}} \int_{-\infty}^{\infty} dx e^{ix\sqrt{\frac{\omega^2}{m^2} - 1} - \frac{2m\bar{\rho}}{\omega^2} x \coth x}, \quad (24)$$

which satisfies the sum rule and coincides with (23) for $\omega - m \gtrsim \bar{\rho}^2/m$.

Next we turn to the case of large densities. The series of infinitely narrow peaks in Eq. (17) stems from the classical picture of the broken translational symmetry of the ground state Eq. (7) which is a periodic lattice of kinks. The true ground state, however, should be translationally invariant, for arbitrarily small β . The symmetry is restored by zero-point fluctuations of the respective positions of kinks in the lattice. Below we show that such fluctuations lead to non-perturbative corrections to Eq. (17) and to the algebraic broadening of the conductance peaks.

In order to analyze finite β corrections to Eq.(17) it is convenient to write the following identity for the correlation function (4)

$$\dot{G}(t) = \int dx \frac{m^2}{\beta} \langle [\sin \beta \phi(x, t), \phi(0)] \rangle, \quad (25)$$

which follows from the equations of motion of the sine-Gordon model. The optical sum rule is taken care of by imposing the initial condition $G(0) = -i$.

With a help of (9) and observing that the ground state solution ϕ_0 satisfies the stationary SG equation we write

$$\dot{G}(t) = \int dx \langle [\phi_0'' \left(x + \frac{\beta\eta(x, t)}{\kappa} \right), \phi_0 \left(\frac{\beta\eta(0)}{\kappa} \right)] \rangle_X \quad (26)$$

where the average over the position of the lattice of kinks X is spelled out explicitly. The function ϕ_0 is a sum of a linear and a periodic function of its argument and can

be represented as a Fourier series

$$\phi_0 \left(x + \frac{\beta\eta}{\kappa} \right) = \frac{\kappa x}{\beta} + \eta + \sum_{l \neq 0} \frac{C_l}{i\beta l} e^{il(\kappa x + \beta\eta)} \quad (27)$$

with $C_l = \text{sech}(\pi l K' / K)$. Using (27) we write Eq. (26) as

$$\dot{G}(t) = \kappa^2 L^{-1} \int dx dy \sum_l C_l^2 e^{i\kappa l(x-y)} Q_l(x-y, t), \quad (28)$$

where

$$Q_l(x-y, t) = \beta^{-2} \langle [e^{il\beta\eta(x,t)}, e^{-il\beta\eta(y)}] \rangle \quad (29)$$

In deriving Eq. (28), off-diagonal terms of the form $\langle [\exp(im\beta\eta(x,t)), \exp(-in\beta\eta(0))] \rangle$ for $n \neq m$ were dropped, since they vanish in the thermodynamic limit. The average over the position of the kink lattice X was replaced by the equivalent integration over y .

The limit $\beta \rightarrow 0$ in (28) is non-trivial because of the long-distance singularities characteristic of this problem. First take this limit naïvely by expanding the exponentials in Eq. (29) in powers of small β and keeping the leading term. Then

$$Q_l(x-y, t) \approx l^2 \langle [\eta(x, t), \eta(y)] \rangle. \quad (30)$$

Using this approximation in formula (28) immediately leads to the peaked structure of the optical response (17).

Next, consider the average commutator in Eq. (29) using the Gaussian approximation

$$\langle e^{i\beta l\eta(x,t)} e^{-i\beta l\eta(0)} \rangle = e^{-\beta^2 l^2 \langle \eta(x,t)\eta(0) \rangle}. \quad (31)$$

Eq. (30) is obtained from the first two terms of the Taylor expansion of the exponential in the right hand side of (31). This expansion is accurate while the argument of the exponential is small, which is not true at large distances, where $\beta^2 \langle \eta(x, t)\eta(0) \rangle \approx \mathcal{K} \log |x^2 - v_s^2 t^2|$,

where \mathcal{K} is the Luttinger parameter,¹⁸. The breakdown of the approximation Eq. (30) at large distances leads to a broadening of the conductance peaks.

A rather lengthy but straightforward analysis, based on Eq. (31) shows then that the real part of optical conductivity near the n -th peak is given by

$$\sigma(\omega_n + \Omega) \propto \sum_l \text{Re} \int_0^\infty dt \frac{l^2 C_l^2 e^{-i\Omega t}}{(\bar{\rho}^2 (v_n^2 - v_s^2) t^2 + 1)^{\mathcal{K} l^2}}, \quad (32)$$

where v_n is the group velocity of the bosonic excitations near frequency ω_n , v_s is the sound velocity of bosonic excitations. We can see, that in the limit $\mathcal{K} = 0$ the delta-function form of the conductivity peak is restored. At any finite value of the Luttinger parameter \mathcal{K} the conductivity will fall off algebraically away from ω_n .

$$\sigma(\omega_n + \Omega) \propto |\Omega|^{2\mathcal{K}-1} \quad (33)$$

The width of the peak, on the other hand, is determined by the difference of the sound velocity v_s and the group velocity v_n and is given by

$$\Delta\Omega = \bar{\rho} \sqrt{v_g^2 - v_n^2} \quad (34)$$

In the high density limit one finds $\Delta\Omega \approx m^2/\rho$ which implies, that peaks of optical conductivity are well resolved despite the quantum smearing of the lattice structure.

In summary, the optical conductivity of a one-dimensional conductor close to the Hubbard-Mott transition in the quasiclassical limit shows a smooth crossover between the Luttinger liquid and the Mott-Hubbard insulator. With increasing density the band of breather absorption splits into a series of well resolved peaks. We calculated the positions of the peaks (19), their shape (33) and width (34). Our analytic result for the Drude weight (21) shows an excellent agreement with the thermodynamic Bethe ansatz.

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